

Quantifying mountain block recharge by means of catchment-scale storage-discharge relationships

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[1] Despite the importance of mountainous catchments for providing freshwater resources, especially in semi-arid regions, little is known about key hydrological processes such as mountain block recharge (MBR). Here we implement a data-based method informed by isotopic data to quantify MBR rates using recession flow analysis. We applied our hybrid method in a semi-arid sky island catchment in southern Arizona, United States. Sabino Creek is a 91 km² catchment with its sources near the summit of the Santa Catalina Mountains northeast of Tucson. Southern Arizona's climate has two distinct wet seasons separated by prolonged dry periods. Winter frontal storms (November–March) provide about 50% of annual precipitation, and summers are dominated by monsoon convective storms from July to September. Isotope analyses of springs and surface water in the Sabino Creek catchment indicate that streamflow during dry periods is derived from groundwater storage in fractured bedrock. Storage-discharge relationships are derived from recession flow analysis to estimate changes in storage during wet periods. To provide reliable estimates, several corrections and improvements to classic base flow recession analysis are considered. These corrections and improvements include adaptive time stepping, data binning, and the choice of storage-discharge functions. Our analysis shows that (1) incorporating adaptive time steps to correct for streamflow measurement errors improves the coefficient of determination, (2) the quantile method is best for streamflow data binning, (3) the choice of the regression model is critical when the stage-discharge function is used to predict changes in bedrock storage beyond the maximum observed flow in the catchment, and (4) the use of daily or night-time hourly streamflow does not affect the form of the storage-discharge relationship but will impact MBR estimates because of differences in the observed range of streamflow in each series.

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1. Introduction

[2] Despite the hydrologic importance of mountainous catchments in providing freshwater resources, especially in semi-arid regions (globally 66.5% of discharge in arid regions comes from mountain catchments) [Viviroli *et al.*, 2007], little is known about key hydrological processes in these systems, such as mountain block recharge (MBR) [Viviroli *et al.*, 2007]. The intrinsic complexity of recharge processes and the fact that such processes are extremely difficult to observe contribute to this problem. Without understanding this key hydrological process in mountainous catchments, assessing the impact of climate variability and

land cover change in these vulnerable systems will be incomplete and possibly inaccurate.

[3] Mountain system recharge (MSR) is the main groundwater recharge component in many arid and semi-arid basins [Wilson and Guan, 2004], and it includes infiltration of mountain stream runoff in alluvial fan streambeds (mountain front recharge, MFR) and precipitation infiltration through mountain bedrock (MBR). Although most studies have focused on recharge processes at the mountain front, a possibly large but unknown contribution of recharge comes from MBR in the sky islands of the southwestern United States [Manning and Solomon, 2003; Blasch and Bryson, 2007].

[4] Understanding the linkage between mountain water sources and basin aquifers is important [de Vries and Simmers, 2002; Scanlon *et al.*, 2006]. MBR influences the mountain groundwater flow system and inter-mountain basin aquifers. Moreover, bedrock groundwater contributes to surface water discharge up to 20%–50% in some systems [Uhlenbrook *et al.*, 2002; Kosugi *et al.*, 2006]. Modeling studies have shown that bedrock permeability and storage capacity have the largest impact on MBR rates [Forster and Smith, 1988; Gleeson and Manning, 2008].

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[5] Various techniques have been used to quantify recharge from mountain systems. These methods range from empirical relationships using annual precipitation, environmental tracers, spatially distributed water balance models, groundwater models, and base flow separation analysis. Empirical equations such as those developed by *Maxey and Eakin* [1949], *Hearne and Dewey* [1988], and *Anderson et al.* [1992] are based on precipitation-recharge relationships, where a certain percentage of precipitation becomes recharge at the mountain front. Recharge in most arid regions is episodic and may be related to large, infrequent, extreme events. As a result, estimating recharge based on a fraction of annual precipitation can be misleading because it ignores the effect of storm characteristics, soil and bedrock storage, and vegetation dynamics on recharge [*Gee and Hillel*, 1988].

[6] Water balance models with various complexities have been used to estimate MBR, but the application of these models is often limited because of the large amount of required input data or model structural deficiencies. For example, *Chavez et al.* [1994] developed an analytical relationship between the mean seasonal precipitation and runoff based on a conceptual understanding of hard rock hydrologic processes for the Sabino Creek catchment, Arizona. The input variables to the model were stochastic, but the model was only developed for the summer season because their analytical streamflow modeling did not consider snowmelt contributions to surface runoff [*Chavez et al.*, 1994]. *Guan* [2005] used the HYDRUS-2D model [*Simunek et al.*, 1999] at the hillslope scale to identify factors that control distributed MBR. He concluded that bedrock permeability, precipitation, potential evapotranspiration, vegetation, and soil coverage control the amount of MBR. Although Guan's model is physically based, it is complex, data intensive, and not well tested with actual observations. He suggested that future efforts should focus on better characterization of hydraulic properties of mountain block and precipitation amounts [*Guan*, 2005]. Detailed field studies at Yucca Mountain, Nevada (60 km²), led to the development of a daily water and energy balance model (INFIL) to estimate spatial variability of net infiltration, which is defined as downward flux across the lower boundary of the root zone [*Hevesi et al.*, 2003]. Capillary forces and temporary perched groundwater systems, which may be important components of streamflow and spring discharge in high mountains, are not considered in this model [*Hevesi et al.*, 2003]. This model was refined to a simpler GIS-based model, the basin characterization model (BCM), which runs at the monthly time step for one soil layer without surface water routing. The BCM developed by *Flint et al.* [2004] provides a method for estimating regional recharge and interbasin comparisons using monthly precipitation, air temperature, potential evapotranspiration, soil water storage, and bedrock permeability [*Flint et al.*, 2004].

[7] *Manning and Solomon* [2003] developed a method using noble gas data to derive recharge temperature, and they distinguished between the sources of MFR and MBR in the Salt Lake Valley Principal Aquifer in northern Utah. They further combined noble gas recharge temperatures, groundwater ages, and temperature data with heat and fluid flow modeling to characterize bulk fluid circulation in the mountain block [*Manning and Solomon*, 2005]. The method

provided useful information regarding the sources of MBR, but its application in other catchments is expensive, and despite measurements at multiple scales, they were unable to determine groundwater circulation depth. Basin groundwater models have also been used to quantify MBR, where MBR is applied as a boundary condition and recharge values are obtained during model calibration. Mountain block recharge estimates from these models are often nonunique [*Manning and Solomon*, 2005]. Recently, isotopic data have been used to constrain MBR estimates in groundwater flow models during model calibration [*Zhu et al.*, 2003; *Sanford et al.*, 2004].

[8] Base flow separation analyses have long been used to estimate groundwater recharge. Although base flow is not entirely recharge, it is often used as a proxy to recharge by assuming that interflow, evapotranspiration (ET), and other losses in the catchment are negligible, and the estimated recharge value is often referred to as base recharge [*Szilagyi et al.*, 2003] or observable recharge [*Holtschlag*, 1997]. *Wittenberg and Sivapalan* [1999] combined base flow separation analysis with inverse nonlinear reservoir routing to estimate groundwater recharge in shallow aquifers of Western Australia while considering ET losses during the summer season only. They assumed a power law relationship between storage and discharge and the slope and intercept of the function derived from series of recession hydrographs that their magnitudes depend on initial recession flow values.

[9] Although many attempts have been made to quantify MBR, less effort has been focused on understanding MBR dynamics in mountainous catchments in relation to precipitation seasonality and catchment storage dynamics. To understand the MBR process, a closer look at catchment storage dynamics and streamflow generation processes is required. *Kirchner* [2009] developed a methodology to quantify catchment dynamic storage based on a streamflow recession analysis method introduced earlier by *Brutsaert and Nieber* [1977]. Catchment dynamic storage is the transient storage of water that discharges during a recession period [*Vitvar et al.*, 2002]. *Kirchner* [2009] used the central tendency of the recession flow data and fitted a regression model to obtain the catchment sensitivity function. The catchment sensitivity function describes the rate of change in discharge as a result of change in storage for periods when precipitation and ET are small relative to discharge. From the sensitivity function one can obtain the storage-discharge relationship for a catchment [*Kirchner*, 2009]. As highlighted by *Teuling et al.* [2010], the work of *Kirchner* [2009] provides a simple framework to explicitly estimate catchment-scale land surface fluxes such as ET and, as shown in this study, MBR using storage-discharge relationships.

[10] Here we introduce a hybrid approach to quantify seasonal MBR based on the catchment storage-discharge relationships proposed by *Kirchner* [2009] and informed by isotope data. The research questions are as follows: (1) How can streamflow recession analysis and isotope data be used to improve understanding of MBR processes in semi-arid mountainous catchments? (2) What is the sensitivity of MBR estimates to uncertainty in the derivation of the catchment storage-discharge relations? (3) What are the contributions of seasonal precipitation (winter versus summer monsoon) to MBR? (4) What can we infer from storage-discharge relations across nested catchments of

increasing size to describe MSR processes in a mountainous catchment?

2. Study Site

[11] The Sabino Creek catchment located in the Santa Catalina Mountains was chosen to represent a sky island catchment and to study MBR processes because of available hydrologic and isotopic data. Marshall Gulch, a 1.5 km² catchment, and Upper Sabino, an 8.8 km² catchment, constitute the headwaters of the Sabino Creek catchment where the majority of MBR occurs (Figure 1). Sabino Creek's drainage area is 91 km², and its elevation ranges from 830 m at the base to 2789 m at Mount Lemmon. Vegetation communities consist of subalpine forest including pine and fir forests in uplands, broadleaf woodland chaparral between 1300 and 2200 m, and desert scrub at the base of the mountain [Whittaker *et al.*, 1968]. The bedrock is mainly leucogranite mixed with gneiss and metasediment and is covered with shallow soils that range in depth from 0.25 m at the base to 1.5 m at higher elevations [DuBois, 1959].

[12] Average annual precipitation is about 300 mm at the base of the mountain and increases to 690–940 mm at the top [Guardiola-Claramonte, 2005]. Precipitation in the catchment is strongly seasonal and includes high-intensity, short-duration storms during the summer monsoon (July–September) and low-intensity, long-duration frontal storms during winter (November–March), with some portion falling as snow at higher elevations. Approximately 50% of the precipitation falls during the summer monsoon season. Air temperature rarely exceeds 32°C in the summer or falls below −5°C in the winter [Brown-Mitic *et al.*, 2007].

3. Our Conceptual Model of Mountain Block Recharge

[13] Understanding MBR processes requires a closer look at precipitation patterns, available energy, and catchment storage dynamics. Our conceptual model of MBR is informed by how catchment storage (in soils above the fractured bedrock and in fractured bedrock) varies in response to precipitation seasonality in headwater catchments and by how streamflow recession analysis across a mountainous system reflects these dynamics of catchment storage and MBR in a hydraulically connected system.

[14] In a typical semi-arid mountainous catchment, the top of the sky islands, with thicker soils, are the major contributor to MBR [Wilson and Guan, 2004]. Lower temperatures and higher precipitation (often in the form of snow) make these areas the principal source of recharge to mountain bedrock aquifers. With the presence of permeable fractured bedrock, precipitation infiltration in sky islands promotes recharge and deep circulation in mountain bedrock aquifers (Figure 2). If the bedrock is relatively impermeable, local flow paths are developed above the bedrock, and thus, most of the recharge originates at the mountain front [Manning and Solomon, 2005].

[15] In the Sabino Creek catchment where bedrock is composed of highly fractured granite and gneiss, we expect to have a hydraulically connected fractured storage system that receives infiltration from sky island catchments (Marshall Gulch and the Upper Sabino Creek). In addition, at certain locations of appropriate topography and geological structure along flow paths, this deep groundwater storage discharges water to streams and springs. While these waters can contribute to recharge at the mountain front, we consider their origin driven by MBR.

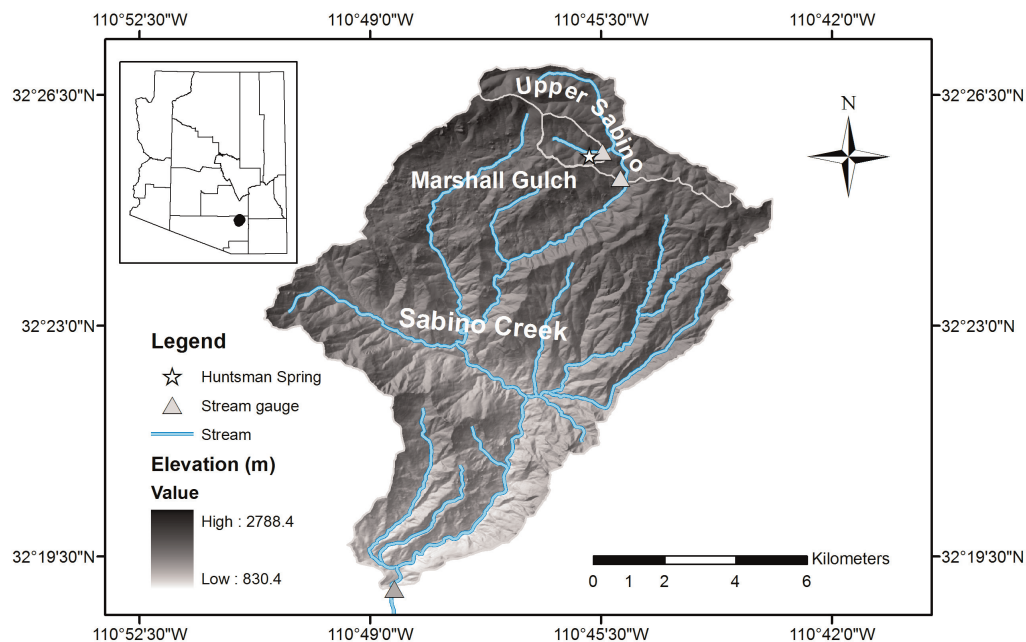


Figure 1. Sabino Creek catchment and its headwaters. The majority of mountain block recharge (MBR) occurs in these headwater catchments where thicker soils are present and subsurface stormflow is an important streamflow generation process [Lyon *et al.*, 2008]. Steep terrain and thin soils on side slopes at lower elevations promote rapid surface runoff, especially during the summer monsoon season.

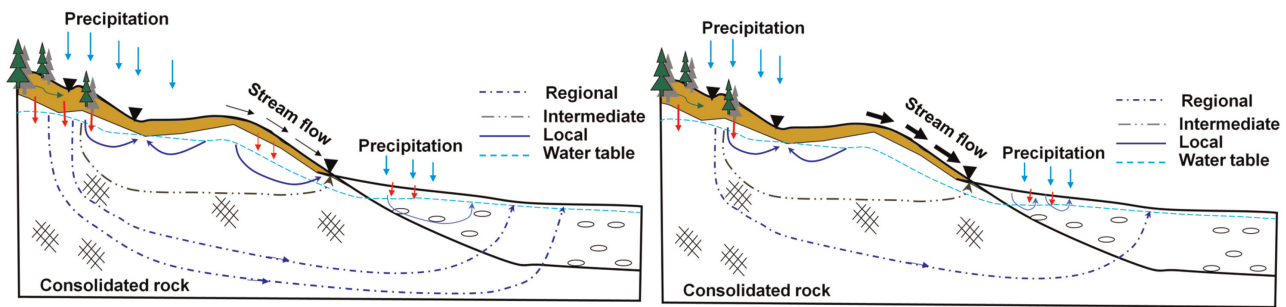


Figure 2. Conceptual model of mountain system recharge processes in a typical semi-arid mountainous catchment with highly permeable fractured bedrock that allows development of deep flow paths. Recharge pathways for each season are shown: (left) winter and (right) summer. Local, intermediate, and regional flow lines are shown. Because of higher winter recharge, all the flow lines are active in the bedrock aquifer (larger zone of lateral subsurface flow). In places where water table intercepts the land surface, streamflows are measured during the dry period. Sky islands with thicker soils and higher precipitation are the main source of MBR to basin aquifers. Steep side slopes at lower elevations promote generation of surface runoff, especially during intense summer rainfall. Surface runoff ultimately reaches the piedmont zone with highly permeable sediment in ephemeral streams and alluvial aquifers. Further recharge at the mountain front occurs as a result of direct infiltration of precipitation through sediments.

[16] While Marshall Gulch and Upper Sabino Creek catchments promote infiltration through thicker soil cover over fractured bedrock, steep terrain with thin soils on side slopes at lower elevations of Sabino Creek promotes rapid surface runoff, especially during the monsoon season. If the surface runoff is large enough, it reaches the piedmont zone and infiltrates through the highly permeable sediments in the stream channel and alluvial aquifer and ultimately contributes to MFR at lower elevations (Figure 2).

[17] In addition to bedrock permeability, precipitation seasonality in the catchment controls the seasonal recharge processes and impacts fractured bedrock storage. Our catchment has two distinct precipitation seasons: winter frontal storms from November to March and summer monsoon convective storms from July to September. These wet periods are separated by prolonged dry periods. During the wet seasons some of the water infiltrates through soils at higher elevations into the fractures of the bedrock, contributing to deep-aquifer storage and raising storage in the fractured system. This storage sustains flow in Marshall Gulch, Upper Sabino, and Sabino Creek during dry periods (April–June and mid-September through early November) where water level in the mountain bedrock intercepts land surface in a hydraulically connected system. Replenishing deep aquifer storage is controlled by soil moisture dynamics that can create shallow saturated zones above bedrock that also allow quick subsurface runoff, especially in the upper part of the mountain system [Lyon *et al.*, 2008]. During dry periods, storage decreases and streamflow drops (lower base flows in early November compared to mid-September and in June compared to April) (Figure 3).

[18] If we are able to estimate storage changes caused by precipitation seasonality in the deep aquifers in fractured bedrock by developing storage-discharge (S - Q) relationships, we have a means to quantify MBR rates. Dynamic storage changes will be estimated simply by measuring changes in base flow prior to and after the precipitation season at a time when all streamflow originates from fractured bedrock discharge. The latter assumes that there is a unique

S - Q relationship that reveals itself using a base flow recession analysis procedure outlined by Brutsaert and Nieber [1977] and Kirchner [2009]. Catchment S - Q relationships derived from recession analysis quantify changes in base flow as a result of change in storage. To get to S - Q functions requires inverting the water balance equation [Kirchner, 2009], which, as will be shown in this study, can be done analytically under certain conditions. After having identified the S - Q relationships, streamflow values before and after a precipitation season are used to obtain change in storage, which we interpret as seasonal MBR. This method of quantifying MBR does not depend on base flow separation as it has been applied previously [Meyboom, 1961; Wittenberg, 1999]. Developing S - Q relations during the dry periods at each of the three gauging stations along Sabino Creek catchment, in conjunction with isotope data, will provide insights about MBR dynamics in a hydraulically connected system.

4. Methods and Materials

[19] We implemented a three-step methodology to quantify MBR processes in mountainous catchments. In the first step, isotope hydrology is used to confirm the above described conceptual model of MBR. Next, catchment storage dynamics in response to precipitation seasonality are investigated by means of recession flow analysis. Finally, storage-discharge relations are developed to quantify MBR rates for those periods in the catchment that change in discharge is only a function of bedrock storage. This methodology is applied at multiple spatial scales in the Sabino Creek catchment corresponding to three gauging stations in Sabino Creek (Figure 1).

4.1. Hydrologic and Isotope Data Collection

[20] Streamflow and precipitation data were obtained for the headwater catchments (Marshall Gulch and Upper Sabino Creek) and Sabino Creek. Marshall Gulch streamflow data includes 2007–2008 streamflow measurements at

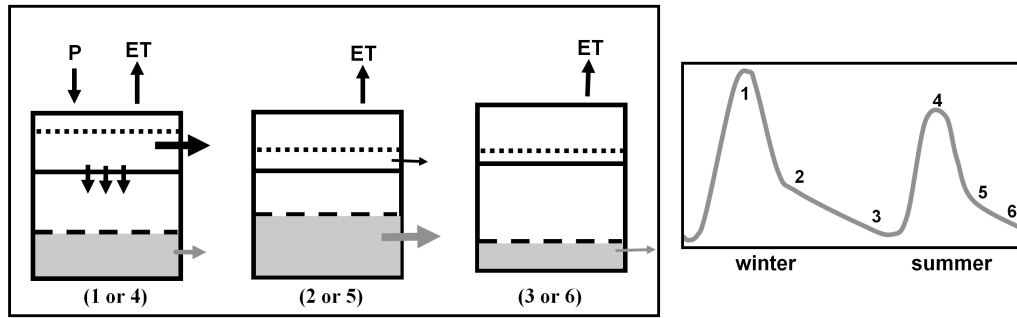


Figure 3. Conceptual diagram illustrating the MBR process during and after rainy periods. In Figure 3 (left), the solid horizontal line indicates the soil-bedrock interface, the dashed line indicates the storage level in the fractured bedrock, and the dotted line indicates the soil moisture storage level. During large storm events, soil moisture storage is filled and contributes some water to the fractured bedrock and replenishes deep aquifer storage (stage 1 or stage 4). Storm hydrographs are composed of surface and shallow subsurface storm runoff and some base flow. In between storm events, surface and subsurface flow ceases, and temporary storage in fractured bedrock releases more water, which constitutes the sole source of streamflow (stage 2 or stage 5 and stage 3 or stage 6). The increase in base flow between stages 3 and 5 and between stages 6 and 2 can be used to estimate dynamic storage increase during wet periods using storage-discharge relationships.

30 min time intervals by the Surface Water Hydrology group of the University of Arizona. Precipitation in the catchment was measured using a series of tipping bucket rain gauges across the catchment [Lyon *et al.*, 2008]. Upper Sabino Creek hourly precipitation and streamflow data were obtained from the Pima County Regional Flood Control District ALERT System (<http://159.233.69.3/perl/pima.pl>) gauge 2290 for 2003–2008. At the base of Sabino Creek, the U.S. Geological Survey (USGS) has a gauging station (ID 09484000) with long-term streamflow records starting in 1932. Daily precipitation and streamflow records from 1988 to 2008 were used in our analysis because of availability of both data sets for that period.

[21] To verify the MBR conceptual model (hydraulic connectivity of the fractured bedrock aquifer and contribution of fractured bedrock to streamflow in dry periods), stable water isotope data of base flow samples (12 samples) for 2006–2008 in Marshall Gulch were used. Additional isotope data including stable water isotopes and tritium data were obtained from previously published [Cunningham *et al.*, 1998; Wright, 2001; Eastoe *et al.*, 2004; Desilets *et al.*, 2008] and unpublished data records for Upper Sabino and Sabino Creek (Table 1). To verify contributions of fractured bedrock to base flow, two water samples were obtained from the Huntsman spring (Figure 1) and Marshall Gulch stream in June 2009 at a time when the soil zone was mostly dry.

Table 1. Summary of Stable Isotope and Tritium Data in the Sabino Creek Catchment

Source	Location	Study
Spring	Santa Catalina Mountains	Cunningham <i>et al.</i> [1998]
Base flow	Marshall Gulch, Upper Sabino, and Sabino Creek	Surface Hydrology Group, Lyon <i>et al.</i> [2008], Desilets <i>et al.</i> [2008]
Groundwater	Mountain front wells	Cunningham <i>et al.</i> [1998], Eastoe <i>et al.</i> [2004]
Precipitation	Palisades Ranger Station	Wright [2001]

4.2. Recession Flow Analysis

[22] Although the recession flow analysis of Brutsaert and Nieber [1977] has been primarily applied to humid catchments [Brutsaert and Nieber, 1977; Zecharias and Brutsaert, 1985; Troch *et al.*, 1993], it has been successfully implemented in the semi-arid region of Mixteca in Mexico. This region is characterized by steep hillslopes with fractured bedrock [Mendoza *et al.*, 2003].

[23] We applied recession flow analyses of Brutsaert and Nieber [1977] for Marshall Gulch to infer catchment storage behavior after precipitation seasons. In this method, streamflow records during rainy days are removed from the data, and changes in daily streamflow between two consecutive days are plotted against the average streamflow on a log-log scale [Brutsaert and Nieber, 1977; Troch *et al.*, 1993; Kirchner, 2009]. The adaptive time stepping method with a time step size of up to 8 days [Rupp and Selker, 2006] was used in the recession analysis to overcome the effects of streamflow measurement errors caused by measurement precision and stage-discharge relations.

[24] To infer the impact of precipitation seasonality on base flow during dry periods, recession flow analyses of Brutsaert and Nieber [1977] were performed for the Marshall Gulch, Upper Sabino, and Sabino Creek while only data from March–June and mid-September to mid-November periods were used. Recession flows during the dry periods that originate from the bedrock aquifer were grouped to post-winter and post-monsoon to examine recession behavior after winter and summer precipitation seasons for the three gauging stations.

4.3. Storage-Discharge Relationship

[25] Changes in the fractured bedrock storage in a catchment over a given time period is described by the conservation of mass equation:

$$\frac{dS}{dt} = P - ET - Q - L, \quad (1)$$

where S [L] is fractured bedrock storage, P [L/T] is precipitation, ET [L/T] is evapotranspiration, Q [L/T] is streamflow, and L [L/T] is lateral subsurface flow from mountain bedrock to regional aquifer. *Kirchner* [2009], on the basis of the catchment water balance equation, showed that in periods when streamflow is only a function of storage in the catchment, the catchment sensitivity function can be obtained from streamflow data. The catchment sensitivity function quantifies change in streamflow as a result of changes in storage:

$$g(Q) = \frac{dQ}{dS} \approx \left. \frac{-dQ/dt}{Q} \right|_{P \ll Q, ET \ll Q}, \quad (2)$$

where $g(Q)$ [T^{-1}] is the catchment sensitivity function.

[26] To derive the catchment sensitivity function of the Marshall Gulch catchment, Upper Sabino, and Sabino Creek, the base flow recession analysis method of *Brutsaert and Nieber* [1977] was performed using daily streamflow data for periods when precipitation and ET are small relative to discharge. Rainy days were removed from daily streamflow data, and only data from March–June and mid-September to mid-November periods were used. These periods correspond to streamflows that originate from fractured bedrock storage in the catchment, and thus, the effect of ET on base flow recession is small. We did not take into account impact of lateral subsurface flow on depleting fractured bedrock storage during dry periods. Therefore, changes in storage during dry periods are solely caused by Q .

[27] Previously, lower envelopes of recession flows have been used to derive catchment storage properties, but there is uncertainty in the exact position of the lower envelop [*Troch et al.*, 1993]. To overcome this uncertainty, *Kirchner* [2009] used the central tendency of the recession flow data to obtain the catchment sensitivity function. The $-dQ/dt$ versus Q data were binned using the quantile method, and only those bins where the standard error $(-dQ/dt) \leq \text{mean}(dQ/dt)/2$ were selected to fit least squares regressions. Stepwise regressions were applied to identify terms based on their statistical significance on the regression model.

[28] The least squares regression model which provides the relationship between dQ/dt and Q in natural log space is the basis for deriving the storage-discharge function. From the catchment sensitivity function $g(Q)$, one can obtain storage-discharge relationships by integrating

$$\int dS = \int \frac{dQ}{g(Q)}. \quad (3)$$

[29] Depending on the form of the least squares regression, $g(Q)$ can have any functional form, and solutions to equation (3) can be obtained analytically or numerically.

[30] If the least squares regression model is linear, the relationship between dQ/dt and Q has the form of a power function:

$$-\frac{dQ}{dt} = aQ^b, \quad (4)$$

where a is the intercept and is related to hydraulic and geomorphic characteristics of the catchment and b is the

recession slope. This functional form was proposed by *Brutsaert and Nieber* [1977], and they showed that the observed hydrograph recession rate as a function of discharge is in good agreement with relationships predicted by Boussinesq's groundwater theory for unconfined aquifers [*Brutsaert and Nieber*, 1977; *Troch et al.*, 1993]. Storage-discharge functions obtained from equation (4) have the form of equation (5) with three classes of solutions, as shown by *Kirchner* [2009]:

$$S - S_0 = \frac{1}{a(2-b)} Q^{(2-b)}. \quad (5)$$

[31] A problem in solving equation (3) arises when $g(Q)$ is in the form of a quadratic polynomial. We developed an analytical solution when $g(Q)$ has the form of a quadratic polynomial with positive quadratic coefficient (concave upward) (Appendix A, equation (A3)). Since S and Q are invertible, by inverting equation (A3), discharge as a function of storage can be obtained (equation (A4)). In the case of a negative quadratic coefficient, equation (3) has to be solved numerically.

[32] Seasonal catchment dynamic storage is obtained by using observed streamflow values before and after a precipitation season in equation (A3) to estimate the maximum observable change in fractured bedrock storage caused by seasonal precipitation, which we interpret as seasonal MBR. The functional relationship in equation (A3) provides a method to estimate MBR:

$$MBR_t = S_{t+1} - S_t = f^{-1}(Q_{t+1}) - f^{-1}(Q_t), \quad (6)$$

where t and $t + 1$ refer to time steps before and after a precipitation season, respectively. Because lateral subsurface flow was not incorporated in our analysis and stream gauging stations may only capture part of the MBR flow path, this method provides the minimum estimate of seasonal MBR.

4.4. Sensitivity Analysis of the Storage-Discharge Function

[33] A series of sensitivity analyses were performed on the Marshall Gulch streamflow values to investigate the impact of (1) streamflow measurement error, (2) data-binning methods, (3) least squares regression model types to represent the storage-discharge functions, and (4) applied time step (daily versus night-time hourly) on storage-discharge functions and subsequent MBR estimation.

[34] Typically, in the *Brutsaert and Nieber* [1977] analysis, the time increment over which the recession slope dQ/dt is calculated is held constant (e.g., 1 day). *Rupp and Selker* [2006] developed a scalable time increment method which takes into account data precision and noise in the data. In this method, the time increment between two recessions is scaled in relation to the streamflow decline. In early recession periods when the drop in discharge is large, small time increments are used, and as recession progresses, the time step of differentiation increases. This method removes horizontal artifacts caused by constant dQ/dt for a range of discharge values often observed in USGS streamflow values [*Eng and Brutsaert*, 1999].

[35] We applied the *Rupp and Selker* [2006] method to investigate the impact of streamflow measurement error, especially during low recession flow periods, on the derived storage-discharge function. In this analysis, first stage-discharge relationships were developed for each gauging station in Sabino Creek. Then the range of errors in stage readings for a given discharge value was calculated on the basis of measured stage data. Using the developed rating curve, discharge values corresponding to the minimum and maximum stage values were calculated, and an error related to a given discharge was estimated. Following *Rupp and Selker* [2006], the time interval to estimate recession slopes for each Q is the value for which the difference between two measured discharges is larger than the threshold value, which is a function of measurement error in the data.

$$Q_{i-j} - Q_i \geq C[Q_{\max} - Q_{\min}], \quad (7)$$

where i is the data point taken at a time step, j is the number of time increments, and C is a constant greater than or equal to 1. Using the corrected Q and dQ/dt data in log-log space, data points were binned, least squares regression equations were fitted, and S - Q functions were derived. Subsequently, the impact of streamflow error on regression model fit and dynamic storage values was evaluated.

[36] There are various ways for data classification and determining class intervals, including equal interval, quantile, and natural breaks methods. We investigated how the selection of a given data-binning technique impacts the S - Q function and ultimately dynamic storage values. We compared the impact of the equal interval and the quantile methods on the S - Q function. In the equal interval method, recession data are binned into a series of groups with an equal range of (log-transformed) streamflow values, and the number of data points in each bin is thus variable. In the quantile method, recession data are grouped in a way that all the bins have the same number of data points. This method will avoid bias toward bins with a larger number of data points. The least squares regression model fitted to binned streamflow values can have any functional form. We analyzed the impact of using linear versus quadratic regression equations on annual MBR values and predicted annual MBR when arbitrary streamflow values beyond observed flows are used.

[37] *Kirchner* [2009] used nightly hourly streamflow data to derive catchment storage-discharge functions. Because high resolution streamflow data are not available for most stream gauges with long-term data records, we analyzed the impact of time step size on deriving storage-discharge functions and subsequent dynamic storage calculations. For the daily streamflow data, streamflow values were converted to an hourly constant rate in order to compare storage-discharge coefficients. For the hourly data, only nightly hourly streamflow values for the dry period were used to develop the S - Q relationship.

5. Results

5.1. Conceptual Model of MBR-Isotopic Evidence

[38] Sabino Creek stable isotope and tritium data across scales illustrate several interesting processes in the catchment that verify our conceptual model, including (1) MBR seasonality, (2) hydraulic connectivity of the bedrock

aquifer, (3) contribution of fractured bedrock storage to streamflow during dry periods at Marshall Gulch, and (4) recharge source areas.

[39] At higher elevations where perennial springs exist, stable isotopes of spring water samples indicate that winter precipitation is the dominant source of water for these springs. Base flow samples from Marshall Gulch and long-term average base flow samples from Upper Sabino Creek (38 samples collected in 1993–2007) also indicate the dominance of winter precipitation [*Desilets et al.*, 2008]. At the lower elevation gauge (Sabino Creek), stable isotopic values of base flow samples in summer indicate that base flow samples have the isotopic composition of Sabino Creek summer precipitation combined with higher elevation winter precipitation samples [*Desilets et al.*, 2008]. These data suggest a continuum of isotopic signatures across the catchment from Upper Sabino Creek base flow that is dominated by winter precipitation to Sabino Creek streamflow that originates from MBR at higher elevations and rainfall-run-off and bank storage processes during summer.

[40] At the mountain front, groundwater samples also indicate dominance of winter precipitation and deeply circulated mountain precipitation in addition to shallow recharge through mountain streams [*Olson*, 1982; *Mohrbacher*, 1984; *Cunningham et al.*, 1998]. Using both O and H stable isotopes in groundwater and precipitation spanning many years, *Eastoe et al.* [2004] confirmed the results of *Simpson et al.* [1970] that the Tucson basin groundwater (which receives waters from the Santa Catalina Mountains, among other mountain ranges) is dominated by winter precipitation recharge.

[41] Tritium data of springs provide evidence about recharge water residence time in the fractured system. Most spring water samples were younger than 50 years, which indicates the presence of a relatively permeable bedrock aquifer with fractures that rapidly transmit water. *Cunningham et al.* [1998] compared stable water isotopic composition of spring samples that plot to the left of the global meteoric water line (GMWL) to mountain stream samples [*Olson*, 1982; *Mohrbacher*, 1984] that plot to the right of the GMWL. Their result indicates rapid infiltration of precipitation and melting snow water before significant losses by evaporation. Moreover, spring water isotope values resembled the deeply circulated fracture flow water of previous studies in the Santa Catalina Mountains [*Cunningham et al.*, 1998].

[42] Stable isotopes of Huntsman spring and Marshall Gulch base flow samples show that both have similar stable isotopic signatures, which suggests contribution of fractured bedrock storage to base flow (Figure 4). Moreover, tritium contents of spring and stream water samples were 4.4 and 3.6 tritium units (1 tritium unit is 1 tritium atom per 10^{18} hydrogen atoms), respectively, which further confirms the similarity of the two waters.

5.2. Storage-Discharge Behavior and Precipitation Seasonality

[43] Average post-precipitation season streamflows are larger in winter compared to summer for Upper Sabino and Sabino Creek catchments because of longer duration precipitation events in winter compared to summer for 2007–2008 (Table 2). In Marshall Gulch, average post-winter

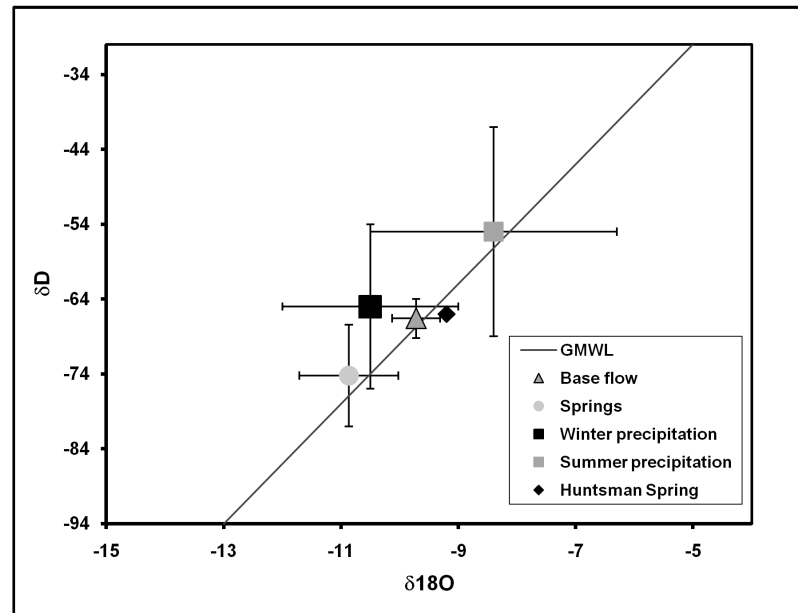


Figure 4. Average value of stable isotopic data of high-elevation springs [Cunningham *et al.*, 1998], Marshall Gulch base flow, and Huntsman Spring during June 2009 in the catchment. Mean stable isotopic data of high-elevation precipitation in winter and summer in Mount Lemmon are shown on the basis of the work of Wright [2001].

recession flows are slightly smaller than the post-monsoon recession flows because of higher summer precipitation in 2007. By June and late October, flow rates in the catchment decrease considerably. At the Sabino Creek gauging station, post-winter flows dominate the recession plot, which indicates a larger contribution of winter recharge to streamflow in the catchment. Post-monsoon recession flows are smaller and exhibit a larger drop in dQ/dt .

5.3. Storage-Discharge Relationships and MBR Rates

[44] For the Marshall Gulch catchment a quadratic model was fit to the daily recession plot in dry periods (Figure 5) because it provided a better fit compared to the linear model (adjusted R^2 value of 0.9 and root-mean-square error (RMSE) of 0.3 mm d^{-2}) (Table 3). Because the catchment sensitivity function has a quadratic form with a positive quadratic coefficient, we applied our analytical solution to derive the S - Q function for Marshall Gulch (equation (8)). Subsequently, by inverting the S - Q function, the Q - S function is obtained (equation (9)).

$$S - S_0 = 17.08 \operatorname{erf}(0.43 \ln Q - 0.57), \quad (8)$$

$$Q = \exp \left\{ \frac{1}{0.43} \left[\operatorname{erf}^{-1} \left(\frac{S - S_0}{17.08} \right) + 0.57 \right] \right\}. \quad (9)$$

[45] For the Upper Sabino and Sabino Creek catchments, a linear model provided a better fit (Figure 6 and Table 4). Using S - Q relations, seasonal MBR values are estimated on the basis of observed streamflow values before and after a precipitation season in each catchment for 2007 and 2008 (Table 5a). Subsequently, average annual MBR values are estimated by adding seasonal MBR rates (Table 5b). Although estimated dynamic storage values that represent MBR rates during this period are smaller in Sabino Creek compared to Marshall Gulch and Upper Sabino, volumetric rates, which are related to catchment area, are much larger.

5.4. Sensitivity Analysis of Storage-Discharge Functions

[46] The impact of streamflow measurement error on the storage-discharge function, regression equation, and streamflow data binning method were investigated, and their impact on adjusted R^2 and RMSE values are presented (Table 6). Our analyses indicate that the Rupp and Selker [2006] correction for the streamflow measurement error lowered RMSE and increased adjusted R^2 values for different model types, especially when the adaptive time step was set up to 8 days. The quantile method decreases RMSE considerably compared to the equal interval classification method. The choice of the regression model is critical when

Table 2. Recession Flow Averages During Dry Periods in All Three Catchments After Winter and Summer Monsoon Precipitation Seasons

Catchment	Post-winter Averages (mm d^{-1})			Post-monsoon Averages (mm d^{-1})		
	2007	2008	Overall	2007	2008	Overall
Marshall Gulch	0.33	0.24	0.29	0.45	0.17	0.31
Upper Sabino	0.24	0.14	0.19	0.019	0.0057	0.012
Sabino Creek	0.055	0.056	0.056	0.0074	0.011	0.0095

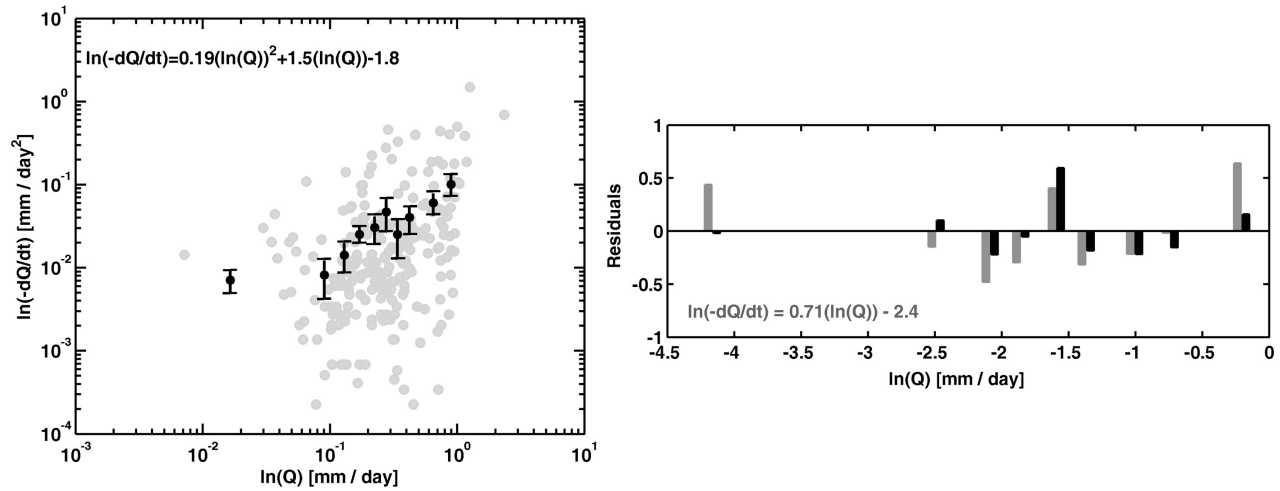


Figure 5. A recession plot for the Marshall Gulch catchment based on daily streamflow data of March–June and mid-September to mid-November (gray dots). Black dots represent binned values obtained using the quantile method, and error bars represent bin standard errors. Standard error of $(-dQ/dt)$ for each bin is less than half of its mean (dQ/dt) . Residuals are shown for both the linear (gray bars) and the quadratic fits (black bars).

the stage-discharge function is used to predict changes in bedrock storage using arbitrary streamflow values beyond the maximum observed flow in the catchment. Using the models in Table 6, annual MBR rates are estimated for Marshall Gulch (Table 7). Estimated annual MBR values based on the observed streamflow data vary between 14.8 and 25.7 mm among different models, while the range for the arbitrary minimum and maximum streamflows is 23.4–46.7. Although different models estimated different MBR rates, values are of the same order of magnitude.

[47] A nightly hourly streamflow data set during the dry period for the Marshall Gulch catchment was used to analyze the impact of streamflow time step on the storage-discharge relationship. No difference was observed in the slope of the Q - S function. The coefficient of the Q - S function for the hourly data is $0.035 \text{ (mm}^{0.2} \text{ h}^{-1}\text{)}$, while for the daily streamflow data converted to constant hourly rate, the coefficient is $0.042 \text{ (mm}^{0.2} \text{ h}^{-1}\text{)}$. Despite the similarity between the coefficients, the estimated annual MBR rates are considerably different (5.1 mm for night-time hourly data compared to 2.9 mm for daily streamflow values in 2008). These differences in annual MBR rates are caused by the difference in observed streamflows before and after a precipitation season for the two times series and are not the result of a different storage-discharge relationship. In 2008,

ratios of minimum night-time hourly streamflow to minimum daily streamflow are 0.9 and 0.4 for winter and summer seasons, respectively. The corresponding ratios for maximum streamflows are 1.1 and 2.1.

6. Discussion

[48] Results presented here demonstrate that streamflow recession analysis provides an indirect method to quantify MBR in semi-arid mountainous catchments. Contrary to the work of *Wittenberg and Sivapalan* [1999], the S - Q functions are directly derived from recession flow data without assuming any specific functional relationship between storage and discharge [*Kirchner*, 2009].

[49] Although our hybrid methodology provides a way to quantify seasonal MBR in mountainous catchments by means of a simple storage-discharge relationship informed by isotopic data, the methodology provides an “inferential tool” as stated by *Kirchner* [2009] for understanding hydrologic behavior, where development of physically based methods requires more data than is usually unavailable. Like any other technique, our approach to quantify MBR is based on certain assumptions, such as low ET rates during dry periods and perennial flow condition at the gauge. However, our approach has several advantages over previous methods to quantify MBR, which may require lots of field observations or information about hydrogeologic properties of the fractured bedrock such as hydraulic conductivity and storativity. Having only streamflow data, one can obtain estimates of MBR by developing S - Q functions, and isotopic data provide valuable information about hydraulic connectivity and contribution of fractured bedrock storage to streamflow during dry period. Despite the method’s simplicity, a series of questions arise upon its application: (1) What are the sources of errors for developing S - Q relationships? (2) Is the estimated MBR based on a dynamic storage value representative of actual recharge

Table 3. Marshall Gulch Regression Models^a

Variables	Linear Model	Quadratic Model
$\ln Q$	0.71 (0.0009)	1.53 (0.003)
$(\ln Q)^2$	N/A	0.19 (0.032)
Intercept	-2.43	-1.8
Adjusted R^2	0.78	0.89
RMSE	0.42	0.30
p value	0.0009	0.0006

^aValues in parentheses are p values. N/A, not applicable; RMSE, root-mean-square error.

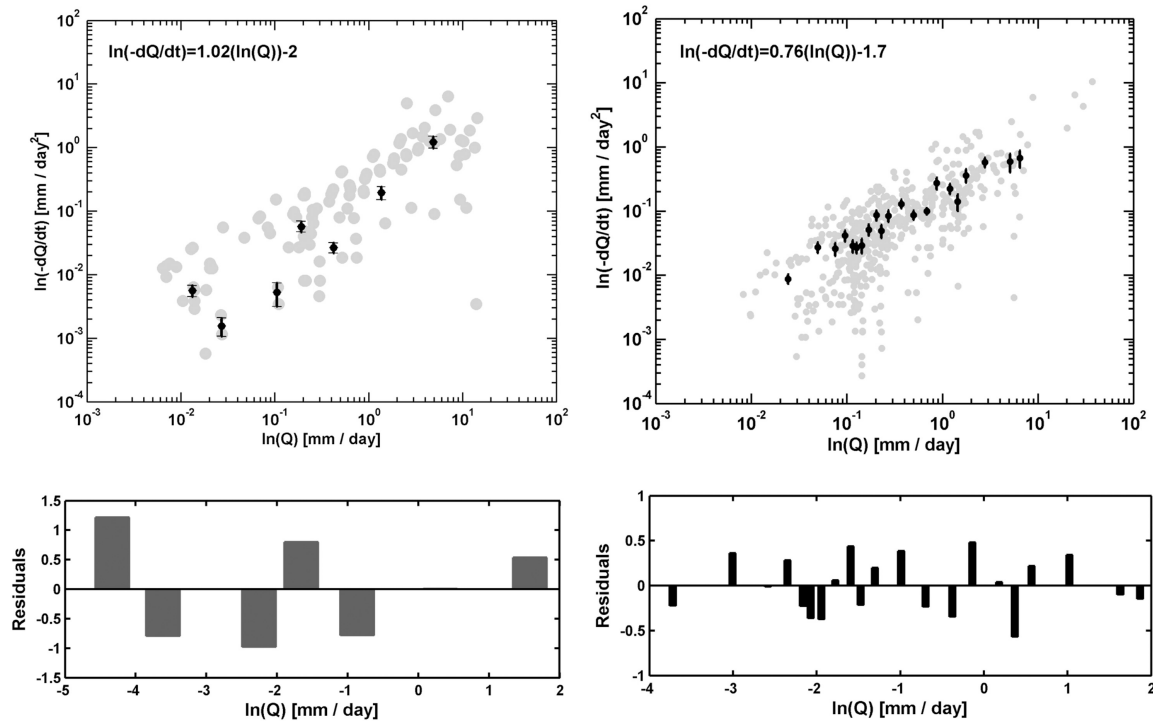


Figure 6. Recession plots for (left) Upper Sabino Creek and (right) Sabino Creek catchments based on daily streamflow data of March–June and mid-September to mid-November (gray dots). Black dots represent binned values obtained using the quantile method, and error bars represent bin standard errors. Standard error of $(-dQ/dt)$ for each bin is less than half of its mean (dQ/dt) .

that occurs in the catchment? (3) Do we expect similar S - Q relationships across the Sabino Creek catchment?

6.1. What Are the Sources of Errors for Developing S - Q Relationships?

[50] Our sensitivity analysis results on Marshall Gulch streamflow data show that streamflow measurement error has a large impact on the model fit, and using the *Rupp and Selker* [2006] method greatly improves model performance. We slightly modified the method to limit the adaptive time step to 8 days. The quantile method is recommended for streamflow classification to remove bias toward bins with a larger number of data values. Although adjusted R^2 values are different on the basis of the regression model type, overall annual MBR values are of the same order of magnitude for Marshall Gulch. The difference in dynamic storage values increase when the linear and quadratic models were used for extrapolation. Other hydrological processes can impact recession flow data and subsequently derived S - Q relationships. For example, at the mountain

front, higher ET rates compared to sky island catchments and bank storage processes introduce uncertainty in Sabino Creek recession data. A larger drop in dQ/dt during the post monsoon period may have been impacted by these processes.

6.2. Is the Estimated MBR Based on a Dynamic Storage Value Representative of Actual Recharge That Occurs in the Catchment?

[51] Our estimates of MBR derived from the S - Q relationships provide a lower-bound estimate of local MBR measured at the gauge. Stream gauging stations may only capture part of the MBR flow path that passes through the catchment and do not capture underflow beneath the gauge. Moreover, the impact of lateral subsurface flow to regional aquifer on depleting fractured bedrock storage is not incorporated in our analysis. Additional isotopic and field measurements need to be collected to provide information about overall mountain bedrock flow paths as outlined in Figure 2.

Table 4. Derived Storage-Discharge Functions for the Upper Sabino and Sabino Creek Catchments

Catchment	Catchment Area (km ²)	S - Q Function	Regression Type	Adaptive Time Step ^a	Adjusted R^2	RMSE
Upper Sabino	8.8	$S-S_0 = 7.71 Q^{0.98}$	Linear	Yes	0.82	0.96
Sabino Creek	91	$S-S_0 = 4.25 Q^{1.24}$	Linear	Yes	0.93	0.32

^aAdaptive time step method of *Rupp and Selker* [2006] was applied to correct for streamflow measurement error.

Table 5a. Observed Streamflow Values Before (Minimum) and After (Maximum) Winter and Summer Precipitation Seasons

Catchment	Winter Q , Minimum, Maximum (mm d ⁻¹)		Summer Q , Minimum, Maximum (mm d ⁻¹)	
	2007	2008	2007	2008
Marshall Gulch	0.054, 1.04	0.27, 2.06	0.0, 1.09	0.045, 0.62
Upper Sabino	0.111, 0.305	0.027, 0.75	0.0, 0.027	0.0, 0.305
Sabino Creek	0.0094, 0.21	0.0, 1.07	0.0, 0.076	0.0, 0.27

6.3. Do We Expect Similar S - Q Relationships Across the Sabino Creek Catchment?

[52] Because the source of streamflow during dry periods in the catchment originates from the fractured bedrock aquifer, we can expect similar S - Q relationships at our three gauging stations. Although streamflow measurement error impacts S - Q coefficients, further differences in coefficients across scales can be explained both by hydraulic theory as presented by *Brutsaert and Nieber* [1977] and by variability theory introduced by *Harman et al.* [2009]. These theories indicate that not only variability in aquifer properties, such as hydraulic conductivity, porosity, hillslope length, and slope impact recession flows, but also seasonal precipitation and inter-storm variability impact S - Q relationships [*Harman and Sivapalan*, 2009]. In the Sabino Creek catchment, additional orographic effects result in different precipitation rates across the catchment that impact local infiltration rates and recession flows. The coefficients of S - Q functions have been previously shown to be related to aquifer properties [*Brutsaert and Nieber*, 1977; *Troch et al.*, 1993]. Because of the complexity of fractured bedrock geometry and the possible violation of other assumptions underlying such relationships at a catchment scale (e.g., homogeneity of aquifer hydraulic properties, hillslope length, and gradient), aquifer properties were not estimated from our recession flow analysis.

[53] In conjunction with streamflow recession analysis, isotopic data were important to confirm our conceptual model of MBR in a semi-arid mountainous catchment and provide information about MBR seasonality and hydraulic connectivity in the catchment. Isotopic data analyses in the catchment demonstrated that winter precipitation is the dominant source of MBR. This result is consistent with precipitation seasonality in the catchment in that we expect higher recharge rates from winter precipitation because of lower intensity, longer duration rainfall and smaller ET

rates. In winter, we expect that local, intermediate, and regional flow lines are more active (i.e., larger zone of lateral subsurface flow). In summer, because of the presence of high intensity storm events, we expect more surface runoff on the side slopes and higher infiltration into the piedmont zone. Therefore, we expect to have more active local flow lines at the mountain front that are generated by bank storage processes in summer. The isotopic signatures of groundwater samples at the mountain front is dominated by winter precipitation, which confirms contribution of regional flow paths in fractured bedrock aquifer to recharge at the mountain front.

[54] Streamflow recession analysis and isotopic data across spatial scales in the Sabino Creek catchment permitted inference of the dynamics of MBR processes in a semi-arid mountainous catchment and emphasized the contribution of headwater catchments to support base flow downstream. Hydraulic connectivity of the bedrock aquifer and topography of the catchment causes interception of the bedrock aquifer water table at the land surface and sustains streamflow at the three gauging stations in the catchment. Estimated dynamic storage values at the three gauging stations permitted a simple mass balance analysis to describe Sabino Creek recharge processes. High elevations (~34% of the catchment) in Sabino Creek are the source areas for MBR because of higher precipitation and a thicker soil zone. On the basis of STATSGO soil depth maps (<http://soils.usda.gov/survey/geography/statsgo/>) the soil depth at higher elevations is ~60 cm. If we assume that the estimated MBR rate at the Upper Sabino Creek catchment is a representative MBR rate for the high elevations and compare it with the total estimated recharge at Sabino Creek catchment, 50% and 72% of MBR estimated from dynamic storage changes at the Sabino Creek catchment originate from the upper elevations for 2008 and 2007, respectively. The rest of the recharge occurs in the lower portion of the watershed, likely because of direct infiltration into the alluvial riparian aquifer and bank storage processes, as was confirmed by isotopic analysis of streamflow samples at the Sabino Creek catchment [*Desilets et al.*, 2008]. Further, stable isotope data and mixing model analysis at the Upper Sabino Creek [*Lyon et al.*, 2008] and Sabino Creek [*Desilets et al.*, 2008] catchments during monsoon events in 2004 and 2006 showed that the concentration of streamflow samples even during large events do not resemble 100% contribution from precipitation end members [*Desilets et al.*, 2008; *Lyon et al.*, 2008]. Therefore, there is a strong base flow component in the system that contributes to streamflow during floods at multiple spatial scales. In the Upper Sabino Creek catchment, after precipitation ceased in the catchment, streamflow samples had pre-event stream water composition [*Lyon et al.*, 2008], while in the Sabino Creek catchment, summer base flow samples have the composition of both winter and summer precipitation [*Desilets et al.*, 2008]. The presence of a strong base flow component originating from high elevations has been previously observed in montane catchments in the United Kingdom using tracers [*Tetzlaff and Soulsby*, 2008]. Capturing this component of the water budget is important for water resources management in alluvial aquifers that are dependent on recharge at high elevations.

Table 5b. Seasonal Mountain Block Recharge (MBR) Values Based on the Observed Streamflow Values in Table 5a

Catchment	Winter MBR (mm)		Monsoon MBR (mm)		Annual MBR (mm)	
	2007	2008	2007	2008	2007	2008
Marshall Gulch	7.2	10.3	7.7	4.5	14.9	14.8
Upper Sabino	1.5	5.6	0.2	2.4	1.7	8.0
Sabino Creek	0.6	4.6	0.2	0.8	0.8	5.4

Table 6. Derived Storage-Discharge Functions for the Marshall Gulch Catchment Using Different Schemes

Model	S - Q Function	Classification Type	Regression Type	Adaptive Time Step ^a	Adjusted R^2	RMSE
1	$S - S_0 = 13.5Q^{0.6}$	Equal interval	Linear	No	0.35	0.96
2	$S - S_0 = 6.13\text{erf}(1.4 \ln Q + 0.88)$	Equal interval	Quadratic	No	0.64	0.71
3	$S - S_0 = 7.7Q$	Equal interval	Linear	Yes	0.51	0.95
4	$S - S_0 = 7.03\text{erf}(0.67 \ln Q + 0.26)$	Equal interval	Quadratic	Yes	0.67	0.78
5	$S - S_0 = 9.8Q^{1.24}$	Quantile	Linear	Yes	0.56	0.57
6	$S - S_0 = 15.09\text{erf}(0.55 \ln Q - 0.36)$	Quantile	Quadratic	Yes	0.63	0.53
7	$S - S_0 = 8.5Q^{1.31}$	Quantile	Linear	Yes	0.78	0.42
8	$S - S_0 = 17.08\text{erf}(0.43 \ln Q - 0.57)$	Quantile	Quadratic	Yes	0.89	0.30

^aLimit Δt to the maximum of 8 days.

7. Conclusions

[55] A hybrid methodology was developed to quantify mountain block recharge processes by means of storage-discharge relations. Storage-discharge relations were developed for the period when fractured bedrock is the only source of water to streamflow. Isotope hydrology was used to confirm our conceptual model of recharge processes across spatial scales in a hydraulically connected catchment.

[56] Sensitivity analysis was performed to show how S - Q functions are influenced by streamflow measurement error, binning procedures, and regression model types. Although the functions have different forms, dynamic storage values estimated on the basis of the observed streamflow values have the same order of magnitude. Problems arise when these functions are used for extrapolation beyond observed streamflow values.

[57] The application of this approach depends on the geologic and hydroclimatic condition of a catchment. Moreover, estimated MBR rates are impacted by simplifying the hydrogeologic conditions of the catchments and certain assumptions involved in development of S - Q relationships. Future efforts should focus on other mountainous catchments to test if similar relationships are observed and how these relationships are impacted by geology, topography, and precipitation seasonality. More detailed experiments can be performed in the presence of detailed information about hydraulic properties of a fractured bedrock aquifer to examine if 3-D modeling approaches and methods that rely on storage-discharge relationships provide similar results.

Table 7. Annual MBR Values Estimated for the Marshall Gulch Using Observed and Arbitrary Minimum and Maximum Streamflows and Different S - Q Functions

Model	Annual Marshall Gulch MBR ^a (mm yr ⁻¹)		Annual Marshall Gulch MBR ^b (mm yr ⁻¹)
	2007	2008	
1	25.7	22.7	39.8
2	22.4	18.6	24.3
3	16.0	18.2	30.7
4	18.6	15.7	23.4
5	20.9	27.3	46.7
6	19.4	19.4	30.3
7	18.3	24.8	42.7
8	14.9	14.8	23.6

^aAnnual MBR rates are estimated on the basis of the observed streamflow values for Marshall Gulch using streamflow values in Table 5a.

^bAnnual MBR rates are estimated on the basis of arbitrary winter flows of 0.01 and 2.5 mm d⁻¹ and summer flows of 0.0 and 1.5 mm d⁻¹ in the catchment.

Appendix A

[58] An analytical solution was developed when the catchment sensitivity function $g(Q)$ obtained from the least squares regression ($-dQ/dt$ as a function of Q) has the form of a quadratic polynomial with positive quadratic coefficient:

$$\begin{aligned} \ln\left(\frac{-dQ}{dt}\right) &= c_1 + c_2 \ln(Q) + c_3 [\ln(Q)]^2, \\ \ln[g(Q)] &= \ln\left(\frac{dQ}{dS}\right) = c_1 + (c_2 - 1) \ln(Q) + c_3 [\ln(Q)]^2, \\ \frac{dQ}{dS} &= \exp\{c_1 + (c_2 - 1) \ln Q + c_3 [\ln(Q)]^2\}. \end{aligned} \quad (\text{A1})$$

[59] Let set $z = \ln Q \rightarrow dQ = \exp(z) dz$,

$$\begin{aligned} dS &= \frac{\exp(z) dz}{\exp[c_1 + (c_2 - 1)z + c_3 z^2]}, \\ \int dS &= \int \exp[-c_1 + (2 - c_2)z - c_3 z^2] dz. \end{aligned}$$

[60] From Abramowitz and Stegun [1972],

$$\begin{aligned} \int e^{-(ax^2 + 2bx + c)} dx &= \frac{1}{2} \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2 - ac}{a}\right) \text{erf}\left(\sqrt{a}x + \frac{b}{\sqrt{a}}\right) \\ &+ \text{const}, \end{aligned} \quad (\text{A2})$$

where erf is the error function: $\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt$. Therefore, the S - Q function has the form:

$$S = \frac{1}{2} \sqrt{\frac{\pi}{c_3}} \exp\left(\frac{(c_2 - 2)^2 - 4c_3 c_1}{4c_3}\right) \text{erf}\left(\sqrt{c_3} \ln Q + \frac{c_2 - 2}{\sqrt{c_3}}\right) + S_0. \quad (\text{A3})$$

[61] Inverting the S - Q function,

$$\begin{aligned} Q &= \exp\left\{\frac{1}{\sqrt{c_3}} \left[\text{erf}^{-1}\left(\frac{S - S_0}{\alpha}\right) - \frac{c_2 - 2}{2\sqrt{c_3}}\right]\right\}, \\ \alpha &= \frac{1}{2} \sqrt{\frac{\pi}{c_3}} \exp\left(\frac{(c_2 - 2)^2 - 4c_3 c_1}{4c_3}\right). \end{aligned} \quad (\text{A4})$$

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